

A generation-based particle-hole density-matrix renormalization group study of interacting quantum dots

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Abstract

The particle-hole version of the density-matrix renormalization-group method (PH-DMRG) is utilized to calculate the ground-state energy of an interacting two-dimensional quantum dot. We show that a modification of the method, termed generation-based PH-DMRG, leads to significant improvement of the results, and discuss its feasibility for the treatment of large systems. As another application we calculate the addition spectrum.

Key words: A. Quantum dots; A. Disordered systems; D. Electron-electron interactions

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1. Introduction

Recently there is a growing interest in the low-temperature physics of disordered many-particle systems, such as electron dephasing due to interactions [1] and the two-dimensional (2D) 'metal-insulator' transition [2]. Transport properties through quantum dots (QDs) have also been recently investigated and shown to exhibit interesting behavior in the presence of both interactions and disorder [3]. An analytical treatment of these problems is unfortunately difficult, since both the disorder and the interactions cannot be considered as a small perturbation. Exact numerical methods for these problems are restricted to small systems, since the size of the many-particle Hilbert space grows exponentially with the system size.

During recent years, several methods were used to decrease the Hilbert space to a size which is computationally feasible. One way is to define an iterative order in which the system is treated, and use a smart

truncation method between the iterations to reduce the space size. This is the idea behind the ensemble of renormalization group methods, such as the numerical renormalization group (NRG) [4] and the density-matrix renormalization group (DMRG) [5].

A different approach uses a predefined constraint in order to truncate. Thus, the entire system may be treated at once, yet not all the system states are taken into account. Therefore, the matrix size one needs to diagonalize is smaller than the entire Hilbert space dimension, and hopefully small enough to be exactly solved. For example, one can approximate the ground state (GS) energy of a system by considering only part of the single-level eigenstates. A sorted list of the eigenstates can be obtained by performing a self-consistent Hartree-Fock (HF) calculation, after which the eigenvectors with the highest eigenvalues are neglected [6]. Such states should, intuitively, have the smallest contribution to the many-particle GS energy.

Another suggestion is based on the localization of the Fock space. Since the interaction term is a two-body operator, only many-body states which differ by at most two electron-hole pairs are cou-

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pled by the Hamiltonian. It was shown [7] that the average contribution of a state containing k electron-hole pairs to the exact GS is proportional to $\exp(-k/\xi_F)$, where ξ_F is the Fock space localization length. Considering also the number of states in the k -th electron-hole generation, $\binom{N-n_e}{k} \binom{n_e}{k}$, where n_e is the number of electrons and N is the number of single-particle states, one finds [6] that the weight of generations falls off exponentially as long as $\xi_F^{-1} > \ln[(N-n_e)n_e/(k+1)^2]$. Thus one can consider in the approximated Hamiltonian only states with a small number of particle-hole (PH) pairs.

In the following we denote these global truncation methods as energy-truncation (ET) and generation-truncation (GT). For a full discussion of both see Ref. [6].

Unfortunately, one cannot simply implement these global truncation methods for larger systems. As the size of the system increases, the number of energy states or PH generations, for a given cutoff, increases, and thus the matrix size increases exponentially, and it soon becomes too large to be solved exactly. Therefore, an alternative method is needed, which can give an accurate approximation to the GS energy, yet can be extended to larger systems. In the following we show that a generation-based PH-DMRG method is suitable for that task.

2. Model

We model the QD as a 2D disordered lattice occupied by n_e spinless electrons. Hopping between nearest neighbors (NNs), and either NN or Coulomb interactions are considered. Therefore, the Hamiltonian can be written as $\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}$, where

$$\hat{H}_0 = \sum_m \epsilon_m \hat{a}_m^\dagger \hat{a}_m - t \sum_{\langle m, n \rangle} (\hat{a}_m^\dagger \hat{a}_n + H.c.), \quad (1)$$

and \hat{H}_{int} is one of the terms

$$\begin{aligned} \hat{H}_{\text{int}}^{(\text{NN})} &= V \sum_{\langle m, n \rangle} \hat{a}_m^\dagger \hat{a}_n^\dagger \hat{a}_n \hat{a}_m; \\ \hat{H}_{\text{int}}^{(\text{C})} &= \frac{1}{2} \sum_{m \neq n} \frac{V_c}{|r_m - r_n|} \hat{a}_m^\dagger \hat{a}_n^\dagger \hat{a}_n \hat{a}_m. \end{aligned} \quad (2)$$

Here, \hat{a}_m^\dagger and \hat{a}_m denote creation and annihilation operators of an electron in lattice site m , $\langle \dots \rangle$ represents NNs, ϵ_m is the on-site energy of site m , chosen randomly from a uniform distribution $[-W/2, W/2]$,

and t is the hopping matrix element between NNs which is conventionally taken as the energy unit. In the interaction terms, V is the NN interaction strength, V_c is the Coulomb interaction in a distance of one lattice unit, and $|r_m - r_n|$ is the distance between sites m and n , measured in lattice units.

The GS energy of the system is calculated using the PH-DMRG method [8]. A detailed description of the specific implementation can be found elsewhere [9]. The general idea of the method is to divide the HF single-particle energy levels to those above (particle-states) and below (hole-states) E_F , and then treat these states iteratively. Starting from the vacuum state, in which all levels below E_F are filled, and all the others are empty, in each iteration one particle-state and one hole-state are added, starting from E_F and proceeding in both directions. The superblock is composed of the states already added, by maintaining the number of particles constant. The superblock diagonalization is followed by a truncation of the Hilbert space of both the particle block and the hole block, using their corresponding density matrices. The iteration ends, and a new couple of states can be added again. The process stops after all of the states were added.

The accuracy of the PH-DMRG method depends mostly on the number of states, p , that are kept between successive iterations. In other words, in each iteration, p eigenvectors of the density matrix are taken, while all the others are neglected. Except the accuracy, p influences dramatically the computational resources required during the process.

In order to compare the PH-DMRG method to other approximations we define the error rate, or the discrepancy, as $D(x) = |x' - x|/|x|$, where x is an exact quantity and x' is an approximation for x . By calculating $\bar{D}(E_{GS})$, averaging over different realizations of the disorder, one thus has a good estimate about the accuracy of the approximation method.

3. Ground-State Energy Calculation

In order to examine the accuracy of the PH-DMRG method we investigate the case of a 4×6 lattice with a disorder strength $W = 5t$, with the same disorder ensemble used in Ref. [6]. In this section we restrict ourselves to the case of NN interactions, with strength $V = 3t$, and use $n_e = 10$.

Typical results, for a specific realization, are shown in Fig. 1(a) (circles), as a function of p , the number of block states kept. The results are com-

pared to the HF results, to the results of the ET method, in which the lowest 18 HF states were used, and to those of the GT method, in which up to 3 PH generations were kept. The exact results are also drawn. As p increases, the PH-DMRG approximation improves.

Averaging over realizations (Fig. 1(b)) (circles) shows that the average accuracy of the PH-DMRG calculation improves very slowly by increasing p . The best PH-DMRG results shown (for keeping 80 states) gets closer to the exact GS than the ET method, yet the GT method is much more accurate.

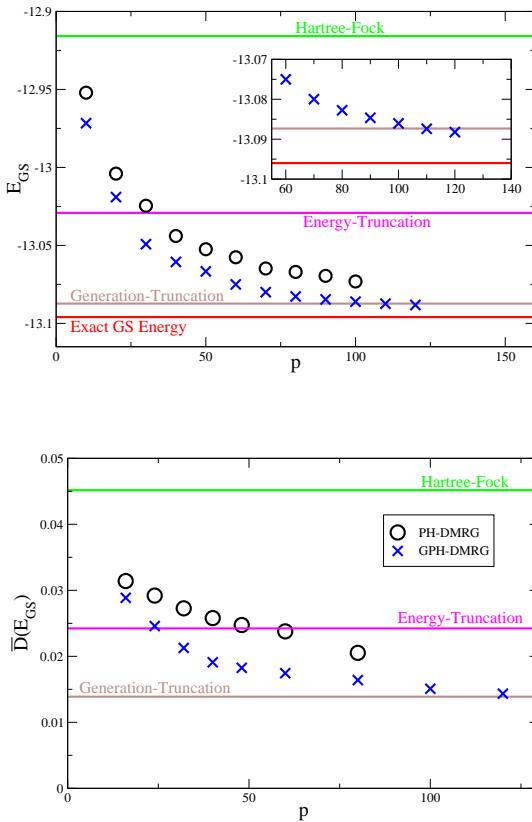


Fig. 1. PH-DMRG results for the GS energy calculation as a function of p (regular version - circles, generation-based version - crosses), compared to various approximated results (see text). (a) The GS energy of a specific realization. Inset: zoom into the region of $p \geq 60$. (b) The discrepancy $\bar{D}(E_{GS}) = \langle |E'_{GS} - E_{GS}| / |E_{GS}| \rangle$ averaged over an ensemble of 100 realizations.

The comparison between the PH-DMRG results and those of the GT method raise the following question: Can one improve the PH-DMRG process without increasing p ? In the following we present such an improvement, motivated by an analysis of the

PH-DMRG truncation method. In essence, the main difference between the DMRG and NRG methods, is the truncation algorithm. In the NRG method, the truncation of states is based on their energies, while in the DMRG it is based on the density-matrix eigenvalues. The density-matrix eigenvectors with the highest eigenvalues are considered as the most important, and the rest of the states are neglected.

Nevertheless, this difference is not the main reason for the DMRG success. This success originates from the fact that while the NRG truncation method is based only on the sites which were already iteratively added, the DMRG algorithm is influenced by additional sites included in the superblock. The superblock is composed of a "system" coupled to an "environment", which represents all the sites which were not yet included in the iteration process, and thus the truncation is based on extrapolation, which leads to better results.

On the other hand, the superblock in the PH-DMRG does not consider any "future" states. The PH-DMRG process couples only the current particle-states and hole-states, but other states are not part of the superblock. Therefore, the truncation does not take them into account, and this limits its success.

In order to improve the truncation decision we suggest to improve the PH-DMRG method by taking into account the number of PH generations as an extra condition taken during the truncation step. As we have discussed above, the idea of the Fock space localization indicates that the weight of successive PH generations decreases exponentially. Therefore, one expects that among states belonging to a given iteration, those with a smaller number of PH generations are more important.

In order to incorporate this criterion into the density-matrix truncation process, we retain all states which contain less than k PH generations in the first round. If there are too many such states, we use the density-matrix eigenvalues, and take the states with the highest eigenvalues. After this first round, if there is still a room for more states, we retain also states with $f > k$, according to their density-matrix eigenvalues, until the maximal number of states p is reached.

For the 4×6 system with 10 electrons, we've executed the suggested truncation method for $k = 0, 1, 2, 3, 4$, and for each realization picked the lowest energy. It turns out, however, that in 95 percents of the samples the $k = 2$ case is the most accurate, so that using a constant $k = 2$ would lead to sim-

ilar results. These results are also shown in Fig. 1 (crosses). As can be clearly seen, the results obtained by the improved method, termed generation-based PH-DMRG (GPH-DMRG), are better by almost 30 percents than the regular PH-DMRG results, and are comparable to the results of the GT method of Ref. [6].

4. Long-range interactions; Strong interactions

The results of the previous section were obtained for short-range interactions. In the framework of the real-space DMRG method there is a huge impact when the interaction range increases. The DMRG iterations add subsequent sites one after another, and if long-range interactions are considered, much more data should be stored from previous steps. Practically, therefore, real-space DMRG applications traditionally consider only short-range interactions.

On the other hand, the interactions range does not affect the GPH-DMRG method almost at all. It does of course change the self consistent HF stage, however, the entire iterations process, which is the most taxing stage of the GPH-DMRG algorithm, remains the same. Thus, one may ask what effect does the interactions range have on the GPH-DMRG accuracy. A related question is how the accuracy is changed when the interactions become stronger.

In Fig. 2 we present the discrepancy between the exact GS and the one obtained by the GPH-DMRG for short-range (upper panel) and long-range (lower panel) interactions. Both strong (filled symbols) and intermediate (empty symbols) interaction strengths are considered. Since these results were obtained for lattices with 6 electrons, i.e., the number of hole-states is small, the accuracy of both the HF approximation and the GPH-DMRG method is better than in the previous section. However, the results show that for both interaction types the GPH-DMRG accuracy is reduced when the interaction strength is enhanced.

A striking feature is the difference in the discrepancy between the short-range and the long-range interactions. For small values of p , the improvement in accuracy of the long-range case is explained by the fact that the HF approximation is better. Nevertheless, the improvement of the long-range results by the GPH-DMRG method is fascinating (\bar{D} for $V_c = 3t$ is reduced by two orders of magnitude), and the averaged discrepancy (for $V_c = 3t$ with $p = 90$

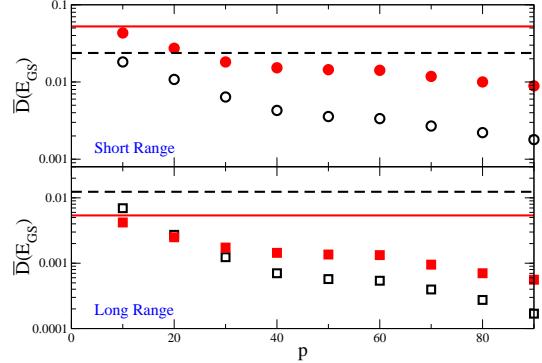


Fig. 2. The discrepancy $\bar{D}(E_{GS})$ obtained by the GPH-DMRG calculation as a function of the number of states kept, for an ensemble of 4×6 disordered lattices occupied by 6 electrons. The accuracy is compared between short-range (upper panel) and long-range (lower panel) interactions, and between intermediate interactions strength ($V = V_c = 3t$, empty symbols) and a strong one ($V = V_c = 10t$, filled symbols). The solid (dashed) lines show the results of the HF approximation for strong (intermediate) interactions. Note the semi-log scale.

states) is $\sim 10^{-4}$, more than an order of magnitude better than the accuracy in the short-range case.

5. Addition Spectrum Calculation

As a useful application of the GPH-DMRG we calculate the addition spectrum of a QD, and compare the discrepancy to that of the HF approximation. The addition spectrum can be defined by

$$\Delta_2 = E_{GS}(n_e) - 2E_{GS}(n_e - 1) + E_{GS}(n_e - 2). \quad (3)$$

Therefore, for a calculation of Δ_2 one needs the GS energies of 3 successive electron numbers for each realization, and we choose the ensemble of 4×6 samples used in the previous sections, occupied by 4, 5 and 6 electrons, with NN or Coulomb interactions. In general, the results are better in the Coulombic case, because of a higher accuracy for each energy calculation.

In Fig. 3 the results for the averaged discrepancy of Δ_2 are presented. The HF approximation obtains, for Coulomb interactions, $\bar{D}(\Delta_2) \approx 1.7$ percents. The GPH-DMRG method, even with a very small number of states ($p \geq 30$), exhibits an improvement of the error rate by more than an order of magnitude, to a level of ~ 0.13 percents.

However, in the NN case the results are quite poor. The starting point of the GPH-DMRG algorithm, i.e., the HF results, give an average error of almost 20 percents. The GPH-DMRG improves it

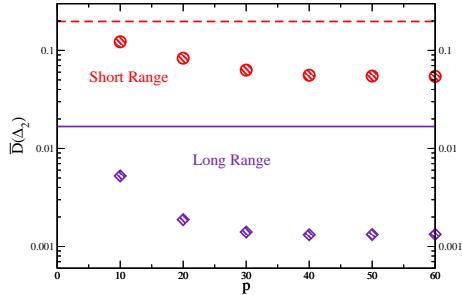


Fig. 3. The averaged discrepancy $\bar{D}(\Delta_2)$ obtained by the GPH-DMRG calculation, for NN (dashed line and circles) and Coulomb (solid line and diamonds) interactions. The GPH-DMRG results are shown in a semi-log scale as a function of p (symbols), together with the HF results (lines).

by a factor of 4, to the order of 5 percent, which is still a very high error rate. It is thus interesting to check whether the calculation of $\langle \Delta_2 \rangle$ and $\delta\Delta_2 = \sqrt{(\Delta_2 - \bar{\Delta}_2)^2}$ are more accurate. These results are shown in Fig. 4.

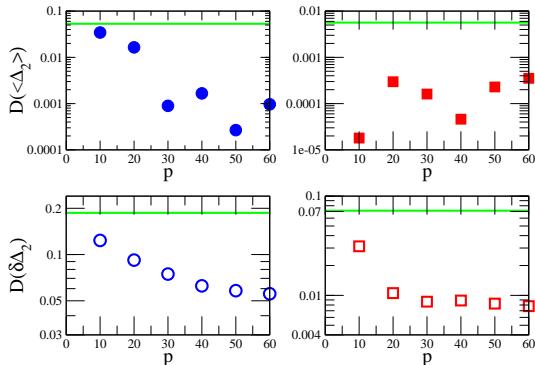


Fig. 4. The GPH-DMRG results for the discrepancy of $\langle \Delta_2 \rangle$ (filled symbols) and $\delta\Delta_2$ (empty symbols) of the 4×6 systems occupied by 4, 5 and 6 electrons with either NN (circles) or Coulomb (squares) interactions. The lines correspond to the HF results.

As can be seen, the results for $\langle \Delta_2 \rangle$ are very accurate for both interaction types, even for very small p . Notice that the results continue to fluctuate around the exact result, since the approximation for Δ_2 is done using 3 different GS approximations, which have different convergence rates. However, for $p \geq 30$, the error is less than 0.1 percent in both cases. The results of $\delta\Delta_2$, on the other hand, show slow convergence. The error rates obtained by the GPH-DMRG (using $p = 60$) for the different cases are

summarized in Table 1. The ratio between the HF discrepancy and that of the GPH-DMRG is shown in parentheses.

	NN	Coulomb
$\bar{D}(\Delta_2)$	0.054314 (3.6)	0.001330 (12.6)
$D(\langle \Delta_2 \rangle)$	0.000965 (55.1)	0.000352 (16.0)
$D(\delta\Delta_2)$	0.055554 (3.4)	0.007794 (9.2)

Table 1
GPH-DMRG error rates for Δ_2 calculation

It is easy to see that for Coulomb interactions the GPH-DMRG improves all results related to the addition spectrum by an order of magnitude, and leads to error rates of less than 1 percent for all cases. However, for the NN interactions, a small error rate and a significant improvement are seen only for $\langle \Delta_2 \rangle$, while modest factors are obtained for $\bar{D}(\Delta_2)$ and $\delta\Delta_2$, with error rates larger than 5 percents.

6. Discussion

In the previous sections we have seen that with an improvement of the truncation algorithm, the GPH-DMRG method can be used for an accurate approximation of the GS energy in disordered systems with interactions. In each of the cases we have checked, the GPH-DMRG led to a significant improvement of the HF results. A comparison to the two methods of Ref. [6] shows that the GPH-DMRG error rate is better than that of the ET method, and is similar to that of the GT one.

Nevertheless, for a full comparison one must also consider the feasibility of these methods when larger systems are treated. To understand the difference between the methods, we compare the matrix sizes for the case considered in section 3. The ET, based on 18 energy levels, and the GT, with up to 3 PH generations, require the diagonalization of matrices of sizes 43, 758 and 47, 916, respectively. The largest superblock Hamiltonian in the GPH-DMRG process, for $p = 120$, is of size 13, 494.

When a larger lattice is studied, and in order to get the same accuracy as for the small system, the ET and GT methods must include more levels and generations. Even was it sufficient to take the same number of levels and generations as in the small case, the size of matrices would have grown exponentially

with the lattice size. Therefore, these methods become infeasible even for modest lattice sizes. In the GPH-DMRG method, on the other hand, the size of the matrix depends on the block size, and not on the system size. Nevertheless, for larger systems, the number of single-particle states is larger, and the discrepancy of the GPH-DMRG is expected to increase, unless p is increased. Therefore, the matrix size being diagonalized is expected to increase in the GPH-DMRG method as well.

The dependence of the largest matrix size needed to be diagonalized in the GPH-DMRG process, M_{max} , on p , is shown in Fig. 5. Although for large values of p , a linear dependence was proposed [10], from our results a power law $M_{max} \sim p^{1.89}$ seems more appropriate. In any case, it is clear that the matrix size is less than quadratic in p . Furthermore, since the largest matrix size used in our current GPH-DMRG application is still much below the technology limit, its increase should not be impossible. It is thus clear that in principle the GPH-DMRG is capable of treating larger systems.

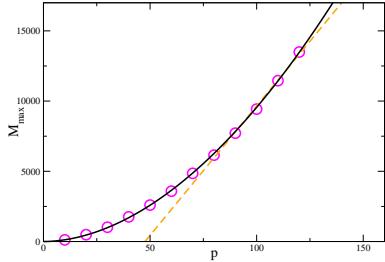


Fig. 5. The maximal size of the superblock Hamiltonian needed to be diagonalized, for the case of section 3. The dashed line is a linear fit of the $p > 80$ points, while the solid line is a power law fit in the entire range.

As a final remark we note that the addition spectrum of disordered QDs with interactions is a long-standing question in mesoscopic physics. Specifically, the behavior of $\delta\Delta_2$ for strong interactions is not completely understood. A comprehensive study of this question was performed a few years ago using the self-consistent HF method [11]. Based on our results, it may thus be relevant to re-examine that question using the GPH-DMRG method.

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